In the Abstract:

Please replace the following abstract for the pending abstract:

Provided is a computer-implemented method of ~~identifying~~ analyzing a macromolecule for potential binding sites ~~on a macromolecule comprising~~ that includes: ~~(a) for at least one organic fragment (ORF), conducting, at separate values of parameter *B*, two or more simulated annealing of chemical potential calculations using the ORF as the inserted solvent;~~ positioning an instance of a computer representation of a molecule or molecular fragment at a plurality of sampling sites of the macromolecule; selecting a value of B, wherein $B = \mu'/kT + ln\langle N\rangle$, where μ' is the excess chemical potential, k is Boltzmann's constant, T is the absolute temperature, and $\langle N\rangle$ is the mean number of molecules of the molecule or molecular fragment; repositioning the instances of the molecule or molecular fragment; accepting or rejecting each instance of the repositioned molecule or molecular fragment based on the Metropolis sampling criteria using the computed binding energy compared to the selected value of B; repeating these steps at a lesser value of B; ~~and (b) comparing converged solutions from step (a) to identify first locations at which the relevant ORF is strongly bound, thereby identifying candidate sites for binding ligand molecules~~ outputting a list of unrejected instances of the molecule or molecular fragment, wherein the molecule or molecular fragment is an organic fragment; and outputting a list of one or more clusters of sampling sites, wherein the clusters of sampling sites include closely located or superimposed sampling sites associated with the unrejected instances of the molecule or molecular fragment.